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Core-Level Photoemission Study of Selfassembled Organic Films on Titanium Oxide Surfaces

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Beamline(s): U12A

Introduction: Alkane phosphonic acids (APAs) can be used to form ordered, covalently bound selfassembled molecular monolayers (SAMs) on native oxide surfaces of titanium and titanium-alloys (such as Ti-6Al-4V). The process believed to yield such layers consists of immersing the substrate in a solution of APA, where a physisorbed SAM forms on the surface. Subsequently, the sample is removed from solution and heated (in air), which leads to the formation of covalent bonds between the phosphonate head group and surface μ-oxo and hydroxyl groups.

Methods and Materials: In order to better understand the exact nature of bonding of APA to the oxide surfaces, core-level photoemission experiments on such samples were carried out at beamline U12A at NSLS. Photoemission (PES) gives information on stoichiometry and local bonding (through chemical shifts) of APA layers on metal oxides. SAMs of octadecylphosphonic acid on Ti and Ti-6Al-4V were prepared ex situ using standard procedures. Subsequently, they were loaded into the ultrahigh vacuum system at U12A to conduct PES experiments.

Results: From the experiments we could conclude that mostly two of the three oxygens of the phosphonate head group are surface bound. Furthermore, angle-dependent PES allowed to confirm that the APA SAMs are highly ordered, *i.e.*, the phosphonate head groups in the film pointing towards the substrate surface. We identified one key obstacle in surface processing to be elongated exposure of the surfaces to ambient conditions, which results in the formation hydrocarbon contamination layers.